ANSYS FLUENT Best Practices

1. Introduction

The following best practices document is provided as courtesy of the HPC Advisory Council.

2. Application Description:

ANSYS FLUENT is a Computational Fluid Dynamics is a computational technology that enables the study of the dynamics of things that flow. Computational Fluid Dynamics (CFD) brings together a number of different disciplines. CFD enables better understanding of qualitative and quantitative physical phenomena in the flow which is used to improve engineering design. ANSYS FLUENT is a leading CFD application from ANSYS. It is widely used in almost every industry sector and manufactured product.

3. Version Information:

ANSYS Fluent 15.0.7

4. System Configuration:

The instructions from this best practice have been tested with the following configuration:

4.1 Hardware:

Dell™ PowerEdge™ R720xd 32 - node (640-core) "Jupiter" cluster

- Dual-Socket Hexa Core Intel E5-2680 V2 @ 2.80 GHz CPUs (Turbo mode enabled Unless otherwise stated)
- Memory: 64GB memory, DDR3 1600 MHz
- OS: RHEL 6.2, OFED 2.3-1.0.1 InfiniBand SW stack
- Hard Drives: 24x 250GB 7.2 RPM SATA 2.5" on RAID 0
- Intel Cluster Ready certified cluster
- Mellanox Connect-IB FDR InfiniBand adapters
- Mellanox ConnectX-3 QDR InfiniBand and Ethernet VPI adapters
- Mellanox SwitchX SX6036 VPI InfiniBand and Ethernet switches
- MPI
  - o Mellanox HPC-X v1.2.0-250, (Provided)
- Application: ANSYS Fluent 15.0.7
- Benchmarks
  - o eddy_417k, turbo_500k, aircraft_2m, sedan_4m, truck_poly_14m, truck_14m
  - o Descriptions for the test cases can be found at the ANSYS Fluent 15.0 Benchmark Page

5. Modifications

ANSYS Fluent provides support for Open MPI as well as for other commercial MPI libraries. The supported version for the Open MPI in Fluent is different from the Open MPI version that is included in the Mellanox HPC-X.

There are minor changes to make HPC-X to work with Fluent. A few steps are shown below to make Mellanox HPC-X working with the existing support in ANSYS Fluent. ANSYS Fluent will support Mellanox HPC-X support in the future ANSYS Fluent releases.

HPC-X is essentially a complete MPI, SHMEM, UPC package, including Mellanox MXM and FCA acceleration engines which offload collectives communication from MPI process onto our interconnect hardware.

5.1 Download the HPC-X distribution:

http://www.mellanox.com/page/products_dyn?product_family=189&mtag=hpc-x

5.2 Add soft links to HPC-X to support running Fluent.

HPC-X is based on OMPI 1.8.2rcX but the libmpi_wrapper.so

For instance, the location could be as follows:

```
/ansys _ inc/v150/fluent/fluent15.0.7/multiport/
mpi _ wrapper/lnamd64/openmpi/libmpi _ wrap-
per.so
```

The libmpi_wrapper.so is a file that Fluent would "dlopen" to get library support from Open MPI. The wrapper for Fluent 15.0.7 was linked with OMPI 1.6.X libraries. Mellanox HPC-X is based on the latest stable release of Open MPI 1.8.x. There needs to be 2 soft links added as stubs in the HPC-X distribution, to make the libmpi_wrapper.so to be able to find the 2 libraries in HPC-X.

At the following location:

```
[root@jupiter001 lib]# pwd
/opt/hpcx-v1.2.0-249-gcc-MLNX_OFED_
LINUX-2.2-1.0.1-redhat6.2/ompi-mellanox-v1.8/
lib
```

The following 2 soft links needed to be created (that needs to be available on each compute nodes):

```
ln -s libopen-rte.so.4 libopen-rte.so
ln -s libopen-pal.so.4 libopen-pal.so
```

5.3 Specifications of MCA parameters

There are a couple of ways to specify the MCA parameters to allow HPC-X to show its best performance by using FCA and MXM. One way to enable MCA parameters in HPC-X is through modifying the mpirun.fl file in fluent, another is to modify the MPIRUN_FLAGS.

The mpirun.fl file is located at `/ansys_inc/v150/fluent/fluent15.0.7/multiport/mpi_wrapper/bin/mpirun.fl`. To enable FCA and MXM for HPC-X explicitly, these lines are added to provide maximum performance on the underlying hardware:

Right around lines 145, I had to add some OMPI specific flags to make both FCA and MXM to work:

```
my_ic_flag+="--map-by node "
my_ic_flag+="-mca coll_fca_enable 1 "
my_ic_flag+="-mca coll_fca_np 0 "
my_ic_flag+="-mca pml yalla "
my_ic_flag+="-mca mtl mxm "
my_ic_flag+="-mca mtl_mxm_np 0 "
my_ic_flag+="-x MXM_TLS=self,shm,ud "
```

The other method is to enable using the MPIRUN_FLAGS environment variable that is set during runtime of Fluent. Below is an example:

```
MPIRUN_FLAGS='--map-by node -mca coll_
fca_enable 1 -mca coll_fca_np 0 -mca
pml yalla -mca mtl mxm -mca mtl_mxm_np
0 -x MXM_TLS=self,shm,ud -x MXM_MPI_
TLS=self,shm,ud'
```

5.4 Specification of Mellanox HPC-X Directory

You also would need to specify the OPENMPI_ROOT to tell Fluent to use an alternate path for Open MPI library instead of the one that is included with Fluent. Below is an example of the HPC-X location used.

```
OPENMPI_ROOT=/opt/hpcx-v1.2.0-249-gcc-ML-
NX_OFED_LINUX-2.2-1.0.1-redhat6.2/ompi-mel-
lanox-v1.8
```

This allows mpirun.fl to pick up to use HPC-X path from my environment variable. The fluent command option `-mpi=openmpi` would allow use the existing Open MPI support to run with Mellanox HPC-X.

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